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Quantum Behaviour And Phonon Emission By Solitons In Crystals At Low Temperature

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Abstract: A rapid increased interest in the behaviour of nonlinear excitations (solitons) and their interactions with each other elementary excitations has been observed recently. In this article this problem is considered in the case of crowdion wave propagation in crystals. However the main results are qualitatively applicable also to kink behaviour in other quasi - one - dimensional systems (polyacetylene, $NbSe_3$ e.t.c) described usually by $\varnothing^4$ and SSH models.

Key words:

INTRODUCTION

As a rule a soliton formation is such systems consists of a number of heavy particles (atoms) and is often treated as a classical particle that is characterized by the position of its mass centre and velocity, V. However, as it was first shown in Pushakarov, D.I., 1973. quantum effects in soliton behaviour happen to be essential in some phenomena. Owing to quantum effects, in particular, no pinning of the soliton to the lattice both in the case of Crowdions and in quasi – one – dimensional structures like polyacetylene can take place in contrast to the predictions of the classical treatment, (Bak, P. and V.L. Pokrovsky, 1981). On the other hand the quantum mechanical description allows to use the well developed mathematical formalism when considering the interactions with each other excitations. Obviously the quantum – mechanical treatment is theorly possible in such problems as phonon emission.

Usually soliton effects are investigated in quasi – one – dimensional structures, i.e. in structures consisting of weakly coupled one – dimensional chains, so that soliton formation arises in each chain independly. A typical example of such a material is polyacetylene, which is studied now intensively. However, in every quasi – one – dimensional structure an interchain interation exists and its effect often is hard to be taken into account. A structure free of such disadvantages is the crowdion. It is a crystal defect caused by an extra atom and arises when the deformation created occurs only in one crystallographic direction (fig. 1). Thus the extra atom is in a more or less close – packed row in which even the remote atoms are displaced from their equilibrium positions. Obviously the crowdion represents as unique example of a one – dimensional structure in a three – dimensional solid. As a rule crowdions are observed in complex lattices along the direction with the minimum period. The crowdion configuration can propagate along this direction and its motion is accomplished owing to small displacements of the atom without any actual migration of the extra atom to the new configuration centre.

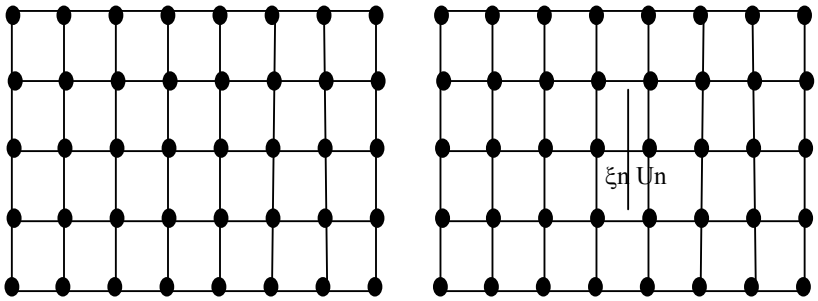

Fig. 1: Crowdion configuration: (a) in an undeformed crystal and (b) in a crystal deformed by an elastic wave.

The model used in (Pushakarov, D.I., 1973). is analogous to the Frenkel – Kontorova dislocation model (Kontorova, T.A. and Ya. I. frenkel, 1938). It is assumed that crowdion atoms interact via elastic forces with their nearest neighbours in the chain and are located in a periodic potential produced by the remaining part of the crystal. If at the same time the crystal is deformed (e.g. due to elastic wave propagation) then the effect of such a deformation amounts to a change in the period and amplitude of this potential.

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Theoretical Considerations and Calculations:

The lagrangian of the system can be written in the form:

$$L = {}^{m}/_{2}\, \Sigma_n U_n^2 - \Sigma_n[mc^2/2(U_{n+1} - U_n)^2 + W(U_n)] \quad (1)$$

where U_n is the displacement of the u^{th} atom its equilibrium position in the ideal lattice, C is the sound velocity in an isolated chain, and W(u) = W(u+1) is the periodic force field produced by the crystal matrix. The lattice constant u=1.

In equation (1) the potential W has been taken in the form

$$W(u) = \tfrac{1}{2} A(1 - \text{Cos } 2\Pi u), \quad (2)$$

and the problem has been reduced to the sine – Gordon model. Having in mind further application to $\varnothing^4$ like models when W(u) is a double well potential of the form shown in fig 2, we shall treat the problem as far as possible in a general way without using the explicit potential form. For the sake for convenience we introduce the notations W(u) = Aw(u), where A is the barrier height between equivalent potential minima

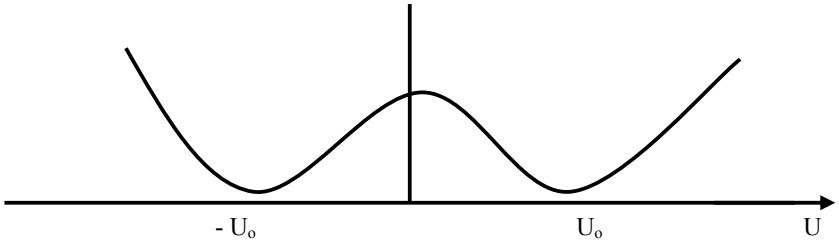

Fig. 2: A double – well potential form used in $\varnothing^4$ and SSH models.

Since we are interested in formations large compared to the lattice constant the equations of motion for the displacements U_n can be written in the continuum approximation limit (in continuous)

$$Mc^2 (1- \beta^2) \frac{\delta^2 U_n}{\delta n^2} = \frac{A\, \delta w,}{\delta U_n} \quad \beta = {}^{v}/_{c} \quad (3)$$

where in addition the solution is supposed to be of the form

$$U_n(t) = U(n - vt) \quad (4)$$

The boundary conditions are

$$\frac{\delta u}{\delta n}\Bigg|_{\pm\infty} = 0,\ u(\infty) = 0$$

$$U(-\infty) = \begin{cases} 1 \text{ for the crowdion} \\ 0 \text{ for } \varnothing^4 \text{ models.} \end{cases}$$

The energy first integral of (3) is

$$\frac{mc^2}{2}(1- \beta^2)\left[\frac{\delta u}{\delta n}\right]^2 = A\, w\,(u) \quad (5)$$

Since the right-hand side w(u) > 0, it follows that v < c.

If V= 0, equation (5) shows that in the continuum limit the strain energy is equal to the energy in the potential W. An increase of V is equivalent to reducing of the strain constant (and hence the strain energy) so that atoms come closer to their equilibrium positions and the length of the configuration becomes smaller.

Taking into account (5) the strain energy, W_e can be written in the form

$$W_e = \frac{mc^2}{2}\int_{-\infty}^{\infty}\left[\frac{\delta u}{\delta n}\right]^2 dn = \frac{mc^2}{2}\int\frac{\delta u}{\delta n}\,du = \frac{1}{2}\,Uo\sqrt{1-\beta^2}, \tag{7}$$

where

$$Uo = \sqrt{2mc^2A}\int_{-uo}^{uo}\sqrt{W(u)}du \text{ and } W(\pm Uo) = W^1(\pm Uo) = 0 \tag{8}$$

In the same way the kinetic energy is found to be

$$\frac{m}{2}\int u_n^2 dn = \beta^2 W_e \tag{9}$$

and the energy connected with the potential W is

$$A\int w(u)dn = \int w(u)\,\frac{dn}{du}\,du = \frac{1}{2}Uo\sqrt{1-\beta^2} \tag{10}$$

Finally, the total energy is

$$E = Uo\sqrt{1-\beta^2} \tag{11}$$

At small velocities ($v << c$) it can be presented as a sum of rest energy, Uo and kinetic energy $½\,\mu v^2$, where

$$\mu = Uo\sqrt{c^2} - m\sqrt{\frac{2A}{mc^2}}\,Uo \tag{12}$$

is the effective mass.

Note, that the contributions of terms (7), (9), (10) to the effective mass μ, are equal in magnitude but differ in sign.

Hence, the soliton energy and effective mass can be found by means only of the potential W (u) without knowing the solution of the equation of motion (3). The existence of a soliton (or soliton-like) solution follows from the fact that the ground state is degenerated with respect to atomic positions in the potential minima.

Using the explicit form of $\varnothing^4$-model potential in conventional notations.

$$W(u) = A\,[(u/u_o)^2 - 1]^2 \,.\, A ¼ yUo^2, \tag{13}$$

one obtains from (8) and (12)

$$U_o = \frac{4mc^2}{3l_o}U_o^2 \tag{14}$$

$$\mu = \frac{4}{3}\,\frac{m}{l_o}U_o^2 - \tag{15}$$

where

$$lo = (2mc^2/\gamma)^{½} \tag{16}$$

The soliton solution of (5) has the simple form

$$U = U_o\,th\,\frac{x + n - nt}{l} \tag{17}$$

Where $l = l_o\sqrt{1-\beta^2}$ is the soliton length, and x is the soliton centre determined by the initial conditions.

Now consider the Crowdion case. The solution of (5) with $W(u) = ½\,(1 - \cos 2\Pi u)$ can be written in the form

$$U(u, t) = {}^{2}/_{\Pi} \operatorname{arctg}\left(e^{\frac{x - n + vt}{e}} \operatorname{tg}\left({}^{\Pi}/_{2}\, u(x)\right)\right) \tag{18}$$

where the soliton length, ρ, is

$$\rho = \rho_o \sqrt{1 - \beta^2}, \quad \rho_o = \sqrt{2mc^2/A}$$

and x is the number of the atoms displaced through the distance u(x). if x is chosen to be the centra\crowdion atom then u(x) =½ and

$$u(n, t) = {}^{2}/_{\Pi} \operatorname{arctg}\left(e^{\frac{x - n + vt}{\rho}}\right) \tag{19}$$

The difference between the displacements of two nearest atoms close to the crowdion centre is

$$u(x+1) - u(x) = \left|{}^{\delta u}/_{\delta n}\right|_x = {}^{1}/_{\Pi}\rho$$

There is a small displacement ${}^{1}/_{\Pi}\rho$ of the central atom, x, leads to a new configuration shifted in a lattice constant and with another central atom, x+1. This is the reason of the small rest energy, U_o, and effective mass, μ, both being proportional to the reciprocal soliton length

$$U_o = 2mc^2/\Pi\rho_o \tag{20}$$

$$\mu = \frac{2}{\Pi} \frac{m}{\rho_o} \tag{21}$$

In the $\varnothing^4$ and SSH-model an additional small parameter $(U_o/a)^2$ occurs due to the small soliton amplitude, U_o, determined by the distance between the nearest equivalent potential minima.

As it has been shown in (Su, W.P.,1980) the soliton effective mass in Polycetylene of the order of the free electron mass. If the soliton is much larger than the lattice constant the solutions (17) and (18) well describe the atomic positions. However, the soliton energy calculated in the continuum approximation is degenerated with respect to the centre position x. The lattice periodicity can be taken into account in good approximation substituting the above solutions into the sum

$$\Sigma = \Sigma_n E_n, \quad E_n = m/2\, u_n^2 + mc^2/2(u_{n+1} - u_n)^2 + W(u_n) \tag{22}$$

Making use of a standard method yields

$$E = \int_{-\infty}^{\infty} dk \sum_{n=-\infty}^{\infty} \delta(n - k)\, E_k = \int_{-\infty}^{\infty} E_k\, d_k + \int E_k \cos 2\Pi k\, d_k + \text{-----} \tag{23}$$

The first integral in the right hand side represents the energy (11). It can be shown that each subsequent integral is smaller by a factor $\exp(-\Pi^2\rho)$. Hence, within a very good approximation one can limit oneself to the second term. The calculation for v=0 yield

$$\delta = ½\, U_1 \cos 2\Pi k, \quad U_1 = \alpha e^{\rho_o}, \tag{24}$$

where the value of the coefficient α depends on the model used. For the sine-Gordon system

$$\alpha_{sG} = 4\Pi^2/9, \tag{25}$$

and for $\varnothing^4$ model

$$\alpha_4 = \delta\Pi^2(\Pi^2/3 - 1)\, \rho_o^2\, U_o^2 \tag{26}$$

Therefore, the soliton moves in a periodic potential with the period of the lattice. The amplitude of this potential, U_1, has been considered in (Bak, P. and V.L. Pokrovsky, 1981) as a pinning energy. From its comparison with the soliton interaction energy the critical soliton concentration necessary for the depinning and "free" soliton propagation has been evaluated. The barrier height, U_1 has been evaluated also in (Su, W.P.,1980) and the conclusion has been made that pinning can take at low temperatures (T< 20 – 40k). An attempt of a

more precise calculation of the pinning energy has been made in (Prelovsek, P. and I. Sega, 1981). However, as it was shown in Pushakarov, D.I., 1973. the pinning of the soliton in such a potential cannot take place even at T=0 due to quantum effects. As a criterion of the quantum behaviour one may use the quantity.

$$\delta = \frac{U_1}{\Pi^2 h^2/\mu a^2}$$

(in a quantum case $\delta \leq 1$). Owing to the small soliton effective mass, μ and exponentially small barrier height, U_1, δ turns out to be smaller than 1 in all physically reasonable cases. In fact, the condition $\delta \leq 1$can be rewritten as

$$\Pi^2 \rho e^{\Pi} \rho \geq \alpha \, (mc^2/\theta_\rho)^2 \, (U_o/a)^2$$

(θ_D being the Debye temperature) which is satisfied even at $\rho=1$.

Hence, the soliton is a quantum particle like an electron in a weak lattice potential. As it has been shown in (Pushakarov, D.I., 1973), it is delocalized and has to be considered as a quasi-particle (soliton wave) that is no longer characterized by the coordinate and velocity of its centre, but by its quasi-wave vector K and dispersion law E(k). Note that as a consequence of the delocalization there is no sense to calculate the "pinning energy" in more detail (taking into account the dependence of the soliton shape on the position of its centre within a unit cell). In fact, tunneling occurs between equivalent states. On the other hand, the contribution to the soliton wave effective mass is negligible.

To find the soliton wave dispersion spectrum of the Schrödinger equation.

$$\Psi'' + \frac{2\mu}{h^2}(E - \tfrac{1}{2}\mu_1 \cos 2\Pi x)\,\Psi = 0$$

that allows solutions of the Bloch-wave form.

$$\Psi = N^{-\frac{1}{2}} e^{kx} \varnothing_k(x)$$

where $\varnothing_k = (x+1) = \varnothing_k(x)$. This spectrum is quite complicated in the general case. However in the case of interest ($\delta << 1$) the dependence of the energy on the quasi-wave vector k can be determined from the following equation Pushakarov, D.I., 1973..

$$\cos K = \cos K_o + \frac{\Pi^2 \delta^2}{4(1-K_o^2/\Pi^2)} \frac{\sin K_o}{K_o}$$

Where $K_o^2 = 2\mu E/h^2$

This leads for small $K_o << 1$ to the dispersion law $E(k) = U_o + \frac{1}{4} U_1 \delta + h^2 k^2/2\mu^*$

where the soliton wave effective mass

$$\mu^* = \mu(1 - (\tfrac{1}{2})\,\delta^2)$$

The wave function at $\delta = 0$ is proportional to the nodeless Mathieu function Ce (x, δ). For $\delta << 1$ it varies slowly and $\delta=0$, Ce (x) =1. Therefore, the wave functions of low-lying soliton excitations can be approximated by place waves.

RESULTS AND DISCUSSION

The consideration made above is obviously restricted by the condition of small soliton velocity V as compared to velocity C called here the sound velocity in the isolated chain. However, as it has been pointed out (Pushakarov, D.I., 1973), the actual sound velocity, S, in complex lattices (the only lattices where crowdions occur) can be drastically different from velocity C. In fact, the sound propagation is connected with displacements of heavy lattice cells containing several atons. On the other hard, the effective strain constant, K, can also be widely different. An illustrative example is a chain with two atoms in a cell and strain constants $K_1 \geq K_2$. Then the effective constant $K = K_1K_2/(K_1+K_2)$ is always smaller than K_1 and in the case $K_1 \geq K_2$ the sound velocity is determined by the smallest constant, K_2.

Therefore, the crowdion can move with a super sound velocity. In this case the propagation of an elastic wave in the crystal amounts to a change in the amplitude A and in the interatomic distances. As a result, the potential W becomes a function of the deformation tensor, Δ:

$$W(U_n, \Delta) = A(\Delta)\,[1 - \cos(2\Pi\, Un - \xi_n / 1+\Delta_1(n))],$$

Where ξn (fig. 1b) is the component of the deformation vector $\vec{\xi}$ along the crowdion chain (chosen as x-axis), $\Delta_1(n) = \xi_{n+1} - \xi_n$. if axial symmetry is assumed, the deformation tensor, Δ, is presented by its three diagonal elements $\Delta_1(n)$, $\Delta_2(n)$, $\Delta_3(n)$. The analysis made is Pushakarov, D.I., 1973. shows that the problem can be fully considered analytically in the most interesting case when the phonon quasi-wave vector components in the crowdion direction are small ($q_x P << 1$). In this case Δ is a function of the crowdion centre and the soliton length takes the form

$$\rho = \frac{1 + \Delta_1}{2\Pi}\sqrt{\frac{\alpha}{2(\Delta)}} = (1+\lambda_1+\Delta_1),$$

where λ_1 are determined by the coefficients in the expression of A in powers of Δ_1:

$$A(\Delta) = A[1 - 2(\lambda_1 - 1)\,\Delta_1 - 2\lambda_2(\Delta_2 + \Delta_3)]$$

As a result, the bottom of the crowdion energy bond is slightly shifted and the crowdion wave can be described by a local dispersion law

$$E(k, \Delta) = U_o + E_1\Delta_1 + h^2k^2/2\mu^*$$

Where $E_1 = U_o(1 - \lambda_1)$, $E_2 = E_3 = \lambda_2(1 - \lambda_1)$.

To consider the phonon emission, the deformation potential method can be used. If the wave propagates along to crowdion chain, the emission probability, W^+, is found to be Pushakarov, D.I., 1973.:

$$W^+ = E^2 / 2h^2M^2N\,(q_y / 2p)[\exp hsq_x /T - 1]^{-1},$$

Where $M = \sum mj$ is the total mass of a lattice cell, $\rho = \mu s q_x/T$ and N is the cell number. Since in this case Phonons with w, w_e vector $q_x - k$ are emitted (or absorbed). $hsq_x (T - hsk/ T - (\Psi s^2/ T)^{1/2}$.

Thus, for $T >> \mu s^2$

$$W^+ = \frac{E^2}{8Ms^2N}\,\frac{q_x}{\mu s}\,\frac{T}{\mu s^2}$$

Conclusion:

If oscillation with all possible directions of the phonon wave $\vec{q}$ are excited in the crystal, then q – T/hs whereas qx – K - $\sqrt{2\mu T/h}$.

Consequently, $q_x/q - (\mu s^2 /T)^{1/2}$ - s/v<< /. Which is typical of the Cherenkov emission cone. In this case, however, the phonon energy can be of the order of the crowdion excitation itself and therefore the process, in general, could be inelastic. It has been recently reported (Bishop, A.R., 1984) about the possibility of super sound propagation of solitons in the SSH model, supported by numerical calculation. But the physical roots of this result seem not to be well understood and are discussed else where.

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